

REPORT DOCUMENTATION PAGE

AFRL-SR-BL-TR-00-

Public reporting burden for this collection of information is estimated to average 1 hour per response, including gathering and maintaining the data needed, and completing and reviewing the collection of information. Send collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Project (0704-0188).

0379

10/1/99

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE November 5, 1999	3. REPORT TYPE AND DATES COVERED Final Technical Report; 5/1/96-11/30/98
4. TITLE AND SUBTITLE High Order Accuracy Computational Methods for Long Time Integration of Nonlinear PDEs in Complex Domains			5. FUNDING NUMBERS F49620-96-1-0150
6. AUTHOR(S) Prof. David Gottlieb			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Division of Applied Mathematics Brown University Providence, RI 02912			8. PERFORMING ORGANIZATION REPORT NUMBER 4
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Office of Scientific Research 801 N. Randolph St., Room 732 Arlington, VA 22031			10. SPONSORING/MONITORING AGENCY REPORT NUMBER
11. SUPPLEMENTARY NOTES			
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release, distribution unlimited			12b. DISTRIBUTION CODE
13. ABSTRACT (Maximum 200 words) The overarching goal of this research was to construct stable, robust and efficient high order accurate computational methods for long time integration of nonlinear partial differential equations. High order accuracy methods (Spectral, Finite Difference and Finite Elements) for the numerical simulations of flows with discontinuities, in complex geometries were developed. In particular applications in supersonic combustion were emphasized. Specific research subjects included: Robust high order compact difference schemes, ENO and WENO schemes, discontinuous Galerkin methods, the resolution of the Gibbs phenomenon, parallel computing and high order accurate boundary conditions. In order to overcome the difficulties stemming from complicated geometries, we have developed multidomain techniques as well as spectral methods on arbitrary grids. Several multidimensional codes for supersonic reactive flows had been constructed as well as a library of spectral codes (Psuedopack).			
14. SUBJECT TERMS			15. NUMBER OF PAGES 19
			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT

Final Report
High Order Accuracy Computational Methods
for Long Time Integration of Nonlinear PDEs
in Complex Domains

AFOSR Grant 96-1-0150
1 May 96 - 30 November 98

David Gottlieb
Division of Applied Mathematics, Brown University
Providence, RI 02912
Phone: (401) 863-2266
Fax: (401) 863-1355
E-mail: dig@cfm.brown.edu

CoPIs:
C.-W.Shu, P.F. Fischer, W.S. Don, J. Hesthaven

20000817 079

1. Objectives:

The main objective of this research was to develop and apply high order accuracy methods (Spectral and Finite Differences) to the numerical simulation of flows with discontinuities, in complex geometries. The prime target of this effort is the simulations of supersonic reactive flows.

The work entailed research in different areas, the results of these converge in the codes developed. Some of these areas are:

- The application of spectral methods to shock wave calculations.
- Development of high order accuracy finite differences ENO and WENO schemes.
- The development of the Discontinuous Galerkin methods.
- The resolution of the Gibbs Phenomenon.
- The developments of high order far field boundary conditions and in particular absorbing layers for aero-acoustic problems.
- General research into the theory of approximations of PDE's.

The above research yielded results that were applied in different problems relevant to US Air-force. As an example we show how to get rid of the oscillations in picture splicing (see later).

2. Summary of Research:

• Spectral Simulations of Supersonic Reactive Flows

The culmination of the research effort under this grant is the construction of a multidimensional spectral code for the simulations of complicated interactions of shock waves and reactive flows. A three dimensional supersonic reactive Navier-Stokes Solver using Chebyshev collocation methods has been used in the study of mixing in a Scramjet engine and addressed the issue of mixing enhancement by shock interactions. The code runs on the IBM-SP2 parallel computer and its accuracy and stability have been

verified. It had been shown that the code provided superior information to low order finite difference schemes.

A new mechanism that might be responsible for breaking up the fuel integrity (enhancing the mixing) was identified. The heavier fluids (H_2O and O_2) are accelerated by the shock penetrating into the lighter fluid (H_2) and tends to form fingers (related to the Richtmyer-Meshkov instability). As the flame jet reaches the other side of the fuel-air interface, a roll-up vortex (related to the Kelvin-Helmholtz instability) is formed at the tip of the flame jet. The flame jet cuts through the hydrogen fuel and makes contact with the air on the other side of the fuel-air interface. The vortex at the tip of the flame jet lifts and breaks up the fuel-air interface. The motion of the vortex creates another flame jet allowing fresh air to penetrate inside and to interact with the fuel. This process repeats itself as the new flame jet reaches the other side of the fuel-air interface.

Low order schemes tend to suppress the formation of the vortex due to its inherently large numerical dissipation. Therefore, the low order scheme predicts the large scale vortical roll-up but not the break-up of the fuel.

The results of this research were reported in [9] and [10].

The filtering techniques developed for this problem has a wide range of applications . In fact in [42] a class of filters based upon the numerical solution of high-order elliptic problems in R^d which allow for independent determination of order and cut-off wave number and which default to classical Fourier-based filters in homogeneous domains were applied. These filters are not restricted to applications in tensor-product based geometries as is generally the case for Fourier-based filters. The discrete representation of the filtered output is constructed from a Krylov space generated in solving a well-conditioned system arising from a low-order PDE.

- Spectral Methods for Complex Geometries:

A major difficulty in the application of high order methods to realistic problems is the issue of applying high-order formulations to complex geometries. Often, generating a reasonable grid around a complex configuration is the most difficult aspect of the solution procedure.

A multi-domain approach based on breaking the geometry into piecewise smooth “sub-domains”, using quadrilaterals (hexahedron) in two (three) dimensions was developed. Each sub-domain is then discretized with a stable tensor product formulation, and the resulting sub-domains are patched together.

It turns out that the most important ingredient of this method is how to impose interface boundary conditions. This is especially important for high order schemes as an improper imposition of those boundary conditions can lead to reduction of accuracy as well as time instabilities. The issue is very subtle as the scheme may still be classically stable, but display non-physical growth in time. We have developed a methodology for a time stable and accurate imposition of interface boundary conditions. It is valid for high-order finite-difference (FD) discretizations and certain spectral formulations. Our method is based on a penalty formulation where the penalty parameters are determined by stability considerations or other properties of the numerical scheme. The SAT procedure assures time stability for systems of equations that have a bounded energy norm. This is not true in general for other high-order FD methods. Indeed, non-penalty approaches often lead to non-physical growth in time for systems of equations, even though the discretization operator is stable for the scalar case. The situation is even more serious for calculations of flows with shock waves. Currently, there are no good methods that can pass shock waves from one sub-domain to the other within high order schemes. A progress had been made for this problem, and at least for the range of strength of shocks relevant to reactive flows, a procedure was developed. For finite difference schemes we had outlined a stable and conservative interface treatment of arbitrary spatial accuracy.

In [3] a method to construct Spectral methods for arbitrary grids was introduced, this extends the validity of the Spectral methods to domains of arbitrary shape. In [32] an optimal set of points for interpolation in triangles were found and using the methodology in [3], an efficient spectral method for triangles was developed in [35].

This advance, together with the multi-domain methodology described above extends spectral methods to complicated geometries.

In [24] the optimal strategy of subdivision of domains for spectral calculations of wave phenomena was discussed. A formula connecting the optimal number of sub-domains with the complexity of the problem (number of waves) and the required accuracy was given. In [20] this was extended to parallel computers, taking the number of processors and communication time into account. It was shown that, for present day multicomputers, the impact of communication overhead does not significantly shift the number of domains and the points at each domain from the optimal uni-processor values, and that the effects of granularity are more important. A different approach to multi-domain methods is considered in [36] where a wavelet optimized adaptive multi-domain method had been presented.

In [28, 29, 33, 34] the penalty method for the multi-domain interface boundary conditions had been presented for the Navier Stokes equations as well as for general hyperbolic equations as the Maxwell's equations for electro-magnetics.

- ENO and Weighted ENO Schemes and Related Topics

We have performed research on high order finite difference and finite volume ENO (essentially non-oscillatory) and WENO (weighted essentially non-oscillatory) schemes. These are schemes suitable for the computation of solutions containing both shocks and other discontinuities and detailed smooth structures.

ENO idea is an adaptive interpolation procedure which tries to automatically choose a locally smoothest region to perform a high order interpolation, hence avoiding crossing a discontinuity whenever possible. WENO is a modification and improvement of ENO schemes. Instead of using only one of the many candidate stencils based on local smoothness as in ENO, WENO uses a linear combination of the contribution from all candidate stencils, each with suitable nonlinear weight.

In [46], Shu and Zeng have applied ENO method to the viscoelastic model with fading memory. The memory term is treated by introducing new variables and rewrite the system by adding more differential equations but without explicit memory terms. The appearance of the memory terms regularizes the solution somewhat, and in many cases it is still a theoretically open question whether shocks will develop from smooth initial data. We have performed theoretical analysis about the linearized system for large time, and have applied ENO scheme to study the nonlinear system for both local time and large time. The high order accuracy and sharp, non-oscillatory shock transition allow us to obtain fine resolution for tens of thousands of time steps, and to study the shock interactions after the formation of shocks.

Application of ENO scheme to the study of shock longitudinal vortex interaction problem is carried out by Erlebacher, Hussaini and Shu in [13]. We have studied the shock/longitudinal vortex interaction problem in axisymmetric geometry. Linear analysis, shock fitting code, and shock capturing ENO are used in different parameter range, to study various cases of nearly linear regime, weakly nonlinear regime, and strong nonlinear regime. Vortex breakdown as a function of Mach number ranging from 1.3 to 10 is studied, extending the range of existing results. For vortex strengths above a critical value, a triple point forms on the shock, leading to a Mach disk. This leads to a strong recirculating region downstream of the shock. It is found out that a secondary shock forms, to provide the necessary deceleration so that the fluid velocity

can adjust to downstream conditions at the shock. Also on ENO schemes, Harabetian, Osher and Shu have investigated a novel Eulerian approach for simulating vortex motion using a level set regularization procedure [27]. Our approach uses a decomposition of the vorticity of the form $\xi = P(\varphi)\eta$, in which both φ (the level set function) and η (the vorticity strength vector) are smooth. We derive coupled equations for φ and η which give a regularization of the problem. The regularization is topological and is automatically accomplished through the use of numerical schemes whose viscosity shrinks to zero with grid size. There is no need for explicit filtering, even when singularities appear in the front. The method also has the advantage of automatically allowing topological changes such as merging of surfaces. Numerical examples including two and three dimensional vortex sheets, two dimensional vortex dipole sheets and point vortices, are given. To our knowledge, this is the first three dimensional vortex sheet calculation in which the sheet evolution feeds back to the calculation of the fluid velocity.

In [40], Jiang and Shu have investigated WENO (weighted ENO) schemes, extending the ideas of Liu, Osher and Chan. In [40], the weights are chosen so that in smooth regions, including at smooth local extrema, they are close to an optimal linear weight which gives the highest possible order of accuracy of an upwind-biased linearly stable scheme. Near shocks, however, those stencils which contain the shock are assigned essentially zero weights. Thus WENO resembles a linear high order upwind biased scheme in smooth regions, and resembles ENO near shocks, with a smooth numerical flux function. One important advantage of WENO, due to its smoothness of fluxes, is that convergence for smooth solutions can be proven. Also, convergence towards steady states is easier than ENO.

Also about high order weighted essentially non-oscillatory (WENO) schemes, jointly with Philippe Montarnal, we have used a recently developed energy relaxation theory by Coquel and Perthame and high order weighted essentially non-oscillatory (WENO) schemes to simulate the Euler equations of real gas [43]. The main idea is an energy decomposition under the form $\varepsilon = \varepsilon_1 + \varepsilon_2$, where ε_1 is associated with a simpler pressure law (γ -law in our case) and the nonlinear deviation ε_2 is convected with the flow.

A relaxation process is performed for each time step to ensure that the original pressure law is satisfied. The necessary characteristic decomposition for the high order WENO schemes is performed on the characteristic fields based on the ε_1 γ -law. The algorithm only calls for the original pressure law once per grid point per time step, without the

need to compute its derivatives or any Riemann solvers. Both one and two dimensional numerical examples are shown to illustrate the effectiveness of this approach.

About high order weighted essentially non-oscillatory (WENO) finite volume schemes on general triangulations, Hu and Shu [37], [38] constructed third and fourth order WENO schemes on two dimensional unstructured meshes (triangles) in the finite volume formulation. The third order schemes are based on a combination of linear polynomials with nonlinear weights, and the fourth order schemes are based on combination of quadratic polynomials with nonlinear weights. We have addressed several difficult issues associated with high order WENO schemes on unstructured mesh, including the choice of linear and nonlinear weights, grouping techniques to avoid negative weights, etc. Numerical examples are shown to demonstrate the accuracies and robustness of the methods for shock calculations.

As a related topic, In [26], S. Gottlieb and Shu further explored a class of high order TVD (total variation diminishing) Runge-Kutta time discretization suitable for solving hyperbolic conservation laws with stable spatial discretizations. We illustrate with numerical examples that non-TVD but linearly stable Runge-Kutta time discretization can generate oscillations even for TVD (total variation diminishing) spatial discretization, verifying the claim that TVD Runge-Kutta methods are important for such applications. We then explore the issue of optimal TVD Runge-Kutta methods for second, third and fourth order, and for low storage Runge-Kutta methods. On another related topic, Perthame and Shu [44] have investigated the issue of positivity preserving (for density and pressure) high order methods for compressible Euler equations of gas dynamics on arbitrary triangulation. A general framework for positivity is established and examples within this framework are given.

- Discontinuous Galerkin Methods

A quite successful technique for hyperbolic conservation laws is the discontinuous Galerkin finite element method. In this method the partial differential equation is multiplied by a test function, integrated over a cell, and formally integrated by parts to obtain a weak formulation. A solution is sought among discontinuous (across cell interface) piecewise polynomials of r -th degree for a $(r + 1)$ -th order method. Because of the discontinuity at cell interface, this method can accommodate successful finite difference methodology (approximate Riemann solvers and limiters) into a finite element framework. Theoretical results similar to finite difference methods, such as total variation stability for 1D and maximum norm stability for 2D and 3D, can be proved for this class of discontinuous Galerkin methods of arbitrary order of accuracy

and for (almost) arbitrary triangulations. An essential difference between this class of finite element method and the finite volume method (which can also be defined on an arbitrary triangulation) is that the latter has only one independent degree of freedom (the cell average) over each cell, while the former has many (for example, it has three degrees of freedom for the piecewise linear case in 2D). This fact renders the scheme more local (no wide stencil reconstruction is needed to compute the flux at cell interface), hence more suitable for parallel computing, and provides a different setting for theoretical justification of stability and convergence of the algorithm. In practice, finite element methods can handle complicated geometry and boundary conditions more easily.

In [6], Cockburn and Shu have studied the Local Discontinuous Galerkin methods for nonlinear, time-dependent convection-diffusion systems. These methods are an extension of the Runge-Kutta Discontinuous Galerkin methods for purely hyperbolic systems to convection-diffusion systems and share with those methods their high parallelizability, their high-order formal accuracy, and their easy handling of complicated geometries, for convection dominated problems. It is proven that for scalar equations, the Local Discontinuous Galerkin methods are L^2 -stable in the nonlinear case. Moreover, in the linear case, it is shown that if polynomials of degree k are used, the methods are k -th order accurate for general triangulations; although this order of convergence is suboptimal, it is sharp for the LDG methods. Preliminary numerical examples displaying the performance of the method are shown.

In [5], Cockburn and Shu have extended the Runge-Kutta discontinuous Galerkin method to multidimensional nonlinear systems of conservation laws. The algorithms are described and discussed, including algorithm formulation and practical implementation issues such as the numerical fluxes, quadrature rules, degrees of freedom, and the slope limiters, both in the triangular and the rectangular element cases. Numerical experiments for two dimensional Euler equations of compressible gas dynamics are presented that show the effect of the (formal) order of accuracy and the use of triangles or rectangles, on the quality of the approximation.

In [2], Atkins and Shu have discussed a discontinuous Galerkin formulation that avoids the use of discrete quadrature formulas. The application is carried out for one and two dimensional linear and nonlinear test problems. This approach requires less computational time and storage than conventional implementations but preserves the compactness and robustness inherent in the discontinuous Galerkin method.

Hu and Shu have presented a discontinuous Galerkin finite element method for solving

the nonlinear Hamilton-Jacobi equations in [39]. This method is based on the Runge-Kutta discontinuous Galerkin finite element method for solving conservation laws. The method has the flexibility of treating complicated geometry by using arbitrary triangulation, can achieve high order accuracy with a local, compact stencil, and are suited for efficient parallel implementation. One and two dimensional numerical examples are given to illustrate the capability of the method. In [41], Lepsky, Hu and Shu have further investigated this method from theoretical and computational points of view. Theoretical results on accuracy and stability properties of the method are proven for certain cases and related numerical examples are presented. It should be noted that for spectral methods, the penalty imposition of boundary conditions is identical with the DG method.

- Psuedopack - Numerical Library for Spectral Differentiations:

A software library using the latest and best algorithms for computing Chebyshev, Legendre and Fourier derivative for multiple data set with optimal accuracy and efficiency was written. This is important since spectral methods based on orthogonal polynomial are very sensitive to roundoff error. Special numerical techniques and algorithms were employed to increase the efficiency and accuracy of the underlining methods.

The package has the following features:

1. Fourier, Chebyshev and Legendre methods on the Gauss-Lobatto points are supported.
2. Matrix-Matrix Multiply Algorithm, Even-Odd Decomposition Algorithm and Fast Fourier/Cosine Transform Algorithm are supported for computing the derivative of a function.
3. Compiled on IBM RS/6000, CRAY, SGI, SUN and Generic UNIX machine.
4. Native fast assembly library call, when available, is used for the library's computational kernel.
5. Special fast algorithms are provided for cases when the function has either even or odd symmetry.
6. Mapping was used to reduce the roundoff error for the Chebyshev and Legendre differentiation.
7. Extensive built-in/User definable coordinate transformation routines.
8. Built-in filtering for smoothing of the function and its derivative.
9. Unified subroutine call interface allows modification of any parameters without any change to be made to the subroutine call statement.

10. Simple user callable subroutines return the derivatives of a multiple data set.

Since the user is shielded from any coding errors of the main derivative routines, reliability of the solutions is enhanced. It speeds up code development, increases productivity and enhances re-usability.

The package is available at www.cfm.brown.edu/people/wsdon/home.html. An early description of the package can be found in [12].

Some of the ideas that were incorporated into the design of this software may be found in [11] where accuracy enhancement for higher derivatives using Chebyshev collocation and a mapping technique is discussed. Also in [7] the accurate computations of high order derivative by spectral methods (known to have troubles with roundoff errors) were discussed.

- Acoustics

Significant progress has been made in the case of plane acoustics embedded in uniform flows. First we tried utilizing the well-behaved PML methods from ambient acoustics in combination with a layer that slowly decelerates the waves to a zero Mach number prior to entering the PML layer, justifying the use of the ambient PML. This is reported in [30] While computations confirm the efficiency and simplicity of the proposed scheme it cannot be claimed to be a true PML method, as the PML property is obtained only for very wide layers. We then applied the methodology based on mathematical method, to develop the first strongly well-posed PML method for the problem of advective acoustics. The additional degrees of freedom, required to ensure the PML property, are introduced through a number of additional ordinary differential equations, and a single partial differential equation. The additional equations are defined so as to ensure that the total set of equations support decaying wave solutions, independent of frequency and angle of incidence of the incoming wave. This research appears in [1].

It is clear that the development of perfectly matched absorbing layers for the equations of acoustics is in its infancy. While the recent encouraging results suggest the possibility of developing such layers for a variety of flow conditions, many important questions remain open.

The work drew the attention of researchers from Pratt and Whitney who are working on the problem of accurate modeling of turbine flutter, where the variable mean flow is obtained from a direct solution of the Euler equations and the noise propagation problem is traced in this mean field using the linearized equations. A joint work is being planned.

- The Resolution of the Gibbs Phenomenon

The nonuniform convergence of the Fourier series for discontinuous functions, and in particular the oscillatory behavior of the finite sum, was already analyzed by Wilbraham in 1848. This was later named *The Gibbs Phenomenon*.

In [22] a review of the Gibbs phenomenon from a different perspective was given. In this view, the Gibbs phenomenon deals with the issue of recovering point values of a function from its expansion coefficients. Alternatively it can be viewed as the possibility of the recovery of local information from global information. The main theme here is not the structure of the Gibbs oscillations but the understanding and resolution of the phenomenon in a general setting.

The purpose of this article was to review the Gibbs phenomenon and to show that the knowledge of the expansion coefficients is sufficient for obtaining the point values of a piecewise smooth function, with *the same order of accuracy as in the smooth case*. This is done by using the finite expansion series to construct a different, rapidly convergent, approximation.

In [23] a general method of extracting high quality approximations from a slowly converging ones have been introduced. Conditions to determine which low order approximation contains enough information such that a better approximation can be derived from it were given. Previous results on the resolution of the Gibbs phenomenon were shown to be special cases of this general theory. This work generalizes and extends the previous work on the Gibbs phenomenon, and the supersonic reactive codes use the theory to overcome the Gibbs oscillation from the shock.

Another application, motivated by a request from R. Albanese (MPD Brooks AFB) of the problem of "gluing" of spliced pictures was considered. A typical situation here is that a two dimensional function $f(x, y)$ is to be determined in a domain $[a \leq x \leq b, c \leq y \leq d]$ from the knowledge of its Fourier coefficients at the non-intersecting sub-domains $[a_i \leq x \leq b_i, c_i \leq y \leq d_i]$. The objective is to approximate the "spliced" function in each sub-domain and then to "glue" the approximations together in order to recover the original function in the full domain.

The Fourier partial sum approximation in each sub-domain yields poor results, due to the Gibbs phenomenon, as the convergence is slow and spurious oscillations occur at the boundaries of *each* sub-domain. Thus once we "glue" the sub-domain approximations back together, the approximation for the function in the full domain will exhibit oscillations throughout the entire domain.

We addressed this problem in one and two dimensions by using techniques developed by us to resolve the Gibbs phenomenon. We have shown that we can "cure" the problem completely for experimental data. The results of this effort are summarized in [18]

- Parallel Computing

A fast direct solver has been developed for parallel solution of "coarse grid" problems, $Au_x = u_b$, such as arise when domain decomposition or multi-grid methods are applied to elliptic partial differential equations in d space dimensions. The approach is based upon a (quasi-) sparse factorization of the *inverse* of A . If A is $n \times n$ and the number of processors is P , our approach requires $O(n^\gamma \log_2 P)$ time for communication and $O(n^{1+\gamma}/P)$ time for computation, where $\gamma \equiv \frac{d-1}{d}$. Results from a 512 node Intel Paragon show that our algorithm compares favorably to more commonly used approaches which require $O(n \log_2 P)$ time for communication and $O(n^{1+\gamma})$ or $O(n^2/P)$ time for computation. Moreover, for leading edge multicomputer systems with thousands of processors and $n = P$ (i.e., communication dominated solves), we expect our algorithm to be markedly superior as it achieves substantially reduced message volume and arithmetic complexity over competing methods while retaining minimal message startup cost. This research is reported in [45].

Efficient solution of the Navier-Stokes equations in complex domains is dependent upon the availability of fast solvers for sparse linear systems. For unsteady incompressible flows, the pressure operator is the leading contributor to stiffness, as the characteristic propagation speed is infinite. In the context of operator splitting formulations, it is the pressure solve which is the most computationally challenging, despite its elliptic origins.

In [14] several preconditioners for the consistent L_2 Poisson operator arising in the spectral element formulation of the incompressible Navier-Stokes equations were examined. A finite element based additive Schwarz preconditioner using overlapping sub-domains plus a coarse grid projection operator which is applied directly to the pressure on the interior Gauss points, was developed. For large two-dimensional problems this approach can yield as much as a five-fold reduction in simulation time over previously employed methods based upon deflation.

As the sound speed is infinite for incompressible flows, computation of the pressure constitutes the stiffest component in the time advancement of unsteady simulations. For complex geometries, efficient solution is dependent upon the availability of fast

solvers for sparse linear systems. In [16] a Schwarz preconditioner for the spectral element method is developed, using overlapping sub-domains for the pressure. These local sub-domain problems are derived from tensor products of one-dimensional finite element discretizations and admit use of fast diagonalization methods based upon matrix-matrix products. In addition, we use a coarse grid projection operator whose solution is computed via a fast parallel direct solver. The combination of overlapping Schwarz preconditioning and fast coarse grid solver provides as much as a fourfold reduction in simulation time over previously employed methods based upon deflation for parallel architectures.

- General Research

It is the nature of research that results in one field can be obtained by research in different fields. Our research led to results in two areas not intended in the proposal.

The Nonlinear Galerkin Method (NGM) was proposed by Temam and was proven to be a powerful tool in approximating complicated dissipative evolution equations.

The method is based on the idea that these equations describe the motion of small scale as well as those of large scales. The method suggest the factorization of the equations to those describing the small scales and those of the large scale. The equation for the small scale are treated differently, since not the small scales themselves are important but rather their influence on the large scales.

It is important for the NGM that it can be cast within the framework of Spectral Methods. This had been done in joint works of Gottlieb and Temam.

In [8] it had been shown that the NGM factorization can be made extremely efficient if different time advancing methods are used for the small scales. Several explicit methods are suggested for the small scales and the savings are outlined.

In [21] the super-convergence of the Galerkin methods for hyperbolic initial boundary value PDE's has been discussed. It was shown that super-convergence is lost as a result of the imposition of boundary conditions. It was also shown that there is no way to recover the super-convergence!!!

In [19] the shape of the sea surface in the steady state solution for a long and narrow basin, as the Gulf of Suez or Baja California, is studied. The study addressed the time-dependent problem encountered when the wind in the wind set-down suddenly relaxes and the water gushes landward under the influence of the pressure gradient force. This is a difficult problem due to a moving singularity associated with the location of the intersection point between the sea surface and the shaping bottom. Spectral methods

as well as finite difference schemes were used. Both codes yielded the same results, the spectral methods with 10 points yielding better results than the MacCormack scheme with 3200 points!! The results indicate that no wave breaking occurs.

3. Personnel Supported

1. David Gottlieb - Ford Foundation Professor.
2. C.-W. Shu - Professor.
3. W.S. Don- Research Professor (full support).
4. P. Fischer- Assistant Professor.
5. J.S. Hesthaven - NSF Postdoctoral Fellow and Assistant Professor.
6. B. Yang, H. Tufo, J. Kruse, C. Hu, A. Gelb - students.

4. Publications and Softwares

References

- [1] S. Abarbanel, D. Gottlieb and J. Hesthaven, *Wellposed perfectly matched layers for advective acoustics*, Journal of Computational Physics, to appear.
- [2] H. Atkins and C.-W. Shu, *Quadrature-free implementation of the discontinuous Galerkin method for hyperbolic equations*, AIAA Journal, v36 (1998), pp.775-782.
- [3] M. Carpenter and D. Gottlieb, *Spectral methods for arbitrary grids*, Journal of Computational Physics, v129 (1996), pp.74-86.
- [4] M. Carpenter, J. Nordstrom and D. Gottlieb, *A Stable and conservative interface treatment of arbitrary spatial accuracy*, Journal of Computational Physics, to appear.

- [5] B. Cockburn and C.-W. Shu, *The Runge-Kutta discontinuous Galerkin method for conservation laws V: multidimensional systems*, Journal of Computational Physics, v141 (1998), pp.199-224.
- [6] B. Cockburn and C.-W. Shu, *The local discontinuous Galerkin method for time-dependent convection-diffusion systems*, SIAM Journal on Numerical Analysis, v35 (1998), pp.2440-2463.
- [7] B. Costa and W.S. Don, *On the computation of high order pseudospectral derivatives*, to appear in Applied Numerical Mathematics (Proceeding of ICOSHAHOM98), 1998.
- [8] B. Costa, L. Dettori, D. Gottlieb and R. Temam *Time stepping for the Nonlinear Galerkin Spectral Methods*, to appear.
- [9] W.S. Don and D. Gottlieb, *High order methods for complicated flows interacting with shock waves*, AIAA Paper 97-0538, 1997.
- [10] W.S. Don and D. Gottlieb, *Spectral simulations of supersonic reactive flows*, SIAM Journal on Numerical Analysis, v35 (1988), pp.2370-2384.
- [11] W.S. Don and A. Solomonoff, *Accuracy enhancement for higher derivatives using Chebyshev collocation and a mapping technique*, SIAM Journal on Scientific Computing, v18 (1997).
- [12] W.S. Don and A. Solomonoff, *PseudoPack v2.3 : Numerical Library for Spectral Differentiation*, 1998.
- [13] G. Erlebacher, M.Y. Hussaini and C.-W. Shu, *Interaction of a shock with a longitudinal vortex*, Journal of Fluid Mechanics, v337 (1997), pp.129-153.
- [14] P. Fischer, *An overlapping Schwarz method for spectral element solution of the incompressible Navier-Stokes equations*, Journal of Computational Physics, v133 (1997), pp.84-101.
- [15] P. Fischer, *Projection techniques for iterative solution of $A\mathbf{x} = \mathbf{b}$ with successive right-hand sides*, Computer Methods in Applied Mechanics and Engineering, v163 (1998).
- [16] P.F. Fischer, N.I. Miller and H.M. Tufo, *An overlapping Schwarz method for spectral element simulation of three-dimensional incompressible flows*, in *Proceedings of the IMA Workshop on Parallel Solution of Partial Differential Equations*, Minneapolis, 1997.

- [17] A. Gelb, *The resolution of the Gibbs phenomenon for spherical harmonics*, Mathematics of Computation, v66 (1997), pp.699-717.
- [18] A. Gelb and D. Gottlieb, *The resolution of the Gibbs phenomenon for splined functions in one and two dimensions*, Computers in Mathematics and Applications, v33 (1997), pp.35-58.
- [19] A. Gelb, David Gottlieb and N. Paldor, *Wind set up relaxation on a sloping beach*, Journal of Computational Physics, v138 (1997), pp.644-664.
- [20] D. Gottlieb and P.F. Fischer, *On the optimal number of subdomains for hyperbolic problems on parallel computers*, International Journal of Supercomputer Applications and High Performance Computing, v11 (1997), pp.65-76.
- [21] D. Gottlieb, B. Gustafsson, P. Olsson and B. Strand, *On the superconvergence of Galerkin methods for hyperbolic IBVP.*, SIAM Journal on Numerical Analysis, v33 (1996).
- [22] D. Gottlieb and C.-W. Shu, *On the Gibbs phenomenon and its resolution*, SIAM Review, v30 (1997), pp.644-668.
- [23] D. Gottlieb and C.-W. Shu, *A general theory for the resolution of the Gibbs phenomenon*, in Atti Dei Convegni Lincei, v147, Tricomi's Ideas and Contemporary Applied Mathematics, Accademia Nazionale dei Lincei, 1998, pp.39-48.
- [24] D. Gottlieb and C.E. Wassberg, *Optimal strategy in domain decomposition spectral methods*. SIAM Journal on Numerical Analysis, to appear.
- [25] S. Gottlieb and P. Fischer, *A modified conjugate gradient method for the solution of $Au = b$ based upon b and $\sqrt{A}b$* , Journal of Scientific Computing, v13 (1998), pp.173-183.
- [26] S. Gottlieb and C.-W. Shu, *Total variation diminishing Runge-Kutta schemes*, Mathematics of Computation, v67 (1998), pp.73-85.
- [27] E. Harabetian, S. Osher and C.-W. Shu, *An Eulerian approach for vortex motion using a level set regularization procedure*, Journal of Computational Physics, v127 (1996), pp.15-26.
- [28] J.S. Hesthaven, *A stable spectral multi-domain method for the unsteady, compressible Navier-Stokes equations*, in Proceedings of The 9'th International Conference on Domain Decomposition, Bergen, Norway, 1996.

- [29] J.S. Hesthaven, *A stable penalty method for the compressible Navier-Stokes equations. II. one-dimensional domain decomposition schemes*, SIAM Journal on Scientific Computing, v18 (1997), pp.658-685.
- [30] J.S. Hesthaven, *Integration preconditioning of pseudospectral operators. I. basic linear operators*, SIAM Journal on Numerical Analysis, v35 (1998), pp.1571-1593.
- [31] J.S. Hesthaven, *On the analysis and construction of perfectly matched layers for the linearized Euler equations*, Journal of Computational Physics, v142, (19??), pp.129-147.
- [32] J.S. Hesthaven, *From electrostatics to almost optimal nodal sets for polynomial interpolation in a simplex*, SIAM Journal on Numerical Analysis, v35, (1998), pp.655-676.
- [33] J.S. Hesthaven, *A stable penalty method for the compressible Navier-Stokes equations. III. multi dimensional domain decomposition schemes*, SIAM Journal on Scientific Computing, to appear.
- [34] J.S. Hesthaven, *Spectral penalty methods*, Applied Numerical Mathematics, to appear.
- [35] J.S. Hesthaven and D. Gottlieb, *Stable spectral methods for conservation laws on triangles with unstructured grids*, Computer Methods in Applied Mechanics and Engineering, to appear.
- [36] J.S. Hesthaven and L. Jameson, *A wavelet optimized adaptive multi-domain method*, Journal of Computational Physics, to appear.
- [37] C. Hu and C.-W. Shu, *High order weighted ENO schemes for unstructured meshes: preliminary results*, Computational Fluid Dynamics 98, Invited Lectures, Minisymposia and Special Technological Sessions of the Fourth European Computational Fluid Dynamics Conference, K. Papailiou, D. Tsahalis, J. Periaux and D. Knorzer, Editors, John Wiley and Sons, v2, September 1998, pp.356-362.
- [38] C. Hu and C.-W. Shu, *Weighted essentially non-oscillatory schemes on triangular meshes*, Journal of Computational Physics, v150 (1999), pp.97-127.
- [39] C. Hu and C.-W. Shu, *A discontinuous Galerkin finite element method for Hamilton-Jacobi equations*, SIAM Journal on Scientific Computing, to appear.
- [40] G. Jiang and C.-W. Shu, *Efficient implementation of weighted ENO schemes*, Journal of Computational Physics, v126 (1996), pp.202-228.

- [41] O. Lepsky, C. Hu and C.-W. Shu, *Analysis of the discontinuous Galerkin method for Hamilton-Jacobi equations*, Applied Numerical Mathematics, to appear.
- [42] *Filtering techniques for complex geometry fluid flows* Comm. in Num. Meth. in Eng. 15, 9-18 (1999).
- [43] P. Montarnal and C.-W. Shu, *Real gas computation using an energy relaxation method and high order WENO schemes*, Journal of Computational Physics, v148 (1999), pp.59-80.
- [44] B. Perthame and C.-W. Shu, *On positivity preserving finite volume schemes for Euler equations*, Numerische Mathematik, v73 (1996), pp.119-130.
- [45] H.M. Tufo and P.F. Fischer, *Fast parallel direct solvers for coarse grid problems*, ANL/MCS Preprint P734-1198 (accepted to J. of Par. & Dist. Comp.).
- [46] C.-W. Shu and Y. Zeng, *High order essentially non-oscillatory scheme for viscoelasticity with fading memory*, Quarterly of Applied Mathematics, v55 (1997), pp.459-484.

5. Technology Transfers

- Gottlieb and Don cooperate closely with A. Nejad and Jeff White from WPAFB on the problem of enhancing mixing by shockwaves. The work continues with Dr. T. Jackson.
- A two dimensional code for subsonic reactive mixing layer was delivered for Nejad's group. The code was written for both Cray and IBM SP2 using MPI. This was a cooperative effort between Nejad, Givi (Buffalo) and our group.
- The code SPARC3D is used in Wright-Patterson Lab. It is an extension of our work on fourth order schemes.
- We have started a joint project with T. Jackson from WPAFB to study recessed cavity flameholders.
- We have close cooperation with J. Shang concerning the construction and application of compact high order schemes.

- We have started a cooperation with Young-Nam Kim from Pratt and Whitney, to implement our PML method for acoustics in modeling of turbine flutter.